Assignment 6

1. In class, we derived the relationship $v_k = \frac{V_k}{N}$ where v_k is the volume of a point in k-space, V_k is the volume of the first Brillouin zone and N is the total number of unit cells in the solid's volume. Show that v_k is also equal to $\frac{(2\pi)^3}{\Omega}$ where Ω is the volume of the unit cell in direct space. Hence the number of k points in the first Brillouin zone (FBZ) does not change by the imposition of a periodic potential.

2. Show that for a Bloch function in 1D

$$\psi_{kn}(x) = e^{ikx} u_{kn}(x), \tag{1}$$

the following Schrodinger equation holds for u_{kn}:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{\hbar}{m} k p_x + V(x) \right] u_{kn}(x) = \left(\varepsilon_n(k) - \frac{\hbar^2 k^2}{2m} \right) u_{kn}(x). \tag{2}$$

3. Consider a simple cubic lattice of a monovalent element. What is the radius of the Fermi sphere k_F relative to the size of the first Brillouin zone (FBZ), k_i? Will distortion of the spherical Fermi surface occur?

4. Consider a BCC monovalent metal. It's primitive lattice vectors are

$$\begin{aligned} \vec{a} &= \frac{a}{2}(1, 1, -1) \\ \vec{b} &= \frac{a}{2}(-1, 1, 1) \\ \vec{c} &= \frac{a}{2}(1, -1, 1) \end{aligned} \tag{3}$$

where $(1, 1, -1)$ represents the vector $\hat{i} + \hat{j} - \hat{k}$ and so on.

(a) Show that the reciprocal lattice vectors are:

$$\begin{aligned} \vec{a^*} &= \frac{2\pi}{a}(1, 1, 0) \\ \vec{b^*} &= \frac{2\pi}{a}(0, 1, 1) \\ \vec{c^*} &= \frac{2\pi}{a}(1, 0, 1). \end{aligned} \tag{4}$$

(b) Construct the first Brillouin zone and show that a dodecahedron (with 12 sides) is formed. Where are the 12 planes in terms of k_x, k_y and k_z?

(c) What is the minimum distance from the origin of the k-space to the nearest zone boundary? Show that the distance is $k_i = \frac{\sqrt{2}\pi}{a}$.

(d) What is the number of electrons per unit volume (n)? Find $k_F = (3\pi^2 n)^{\frac{1}{3}}$ where k_F shows the size of the Fermi sphere.

(e) Find $\frac{k_F}{k_i}$. How far or close to the zone boundaries does the Fermi surface extend?

(f) Repeat all the above calculations for a monovalent FCC metal. Which of the FCC or BCC lattices is more likely to have a distorted Fermi sphere?